02.1-06 CRYSTALLOGRAPHIC STUDIES OF THE 2Fe FERREDOXIN FROM *HALOBACTERIUM* OF THE DEAD SEA By: J.L. Sussman, M. Harel and A. Yonath, Department of Structural Chemistry, Weizmann Institute of Science, Rehovot, Israel.

Bacteria of the genus *Halobacterium* are obligate halophiles, i.e. they require for their growth an extracellular salt concentration higher than 2M NaCl. In fact, they pump in salt, so that their internal salt concentration is higher than that of the environment. It is surprising that halophilic proteins can function under such hostile conditions whereas most other proteins are inactive. Upon lowering the salt concentration in vitro, most of the halophilic enzymes are inactivated. A detailed three-dimensional molecular structure of a halophilic protein can provide some insight to explain this phenomenon.

Crystals of 2Fe-2S ferredoxin from *Halobacterium* of the Dead Sea have been grown in 3.8M phosphate buffer pH = 7.0 . The crystals belong to space-group $P6_322$ with cell dimensions of a=b=60.3 Å c=127.5 Å. In order to prolong the crystals' life-time under X-ray radiation the mother liquor was saturated with styrene monomer. This enabled the collection of complete data sets from single crystals.

X-ray data were collected on a CAD4 diffractometer using monochromated CuKα radiation. From two crystals, independent native data sets for the unique 1/24 of the sphere of reflection were collected, together with Friedel pairs out to 2.4 Å resolution, with a maximum intensity decay of 20%.

One heavy-atom derivative - $K_2Pt(CN)_4^=$ - data set was collected in a similar way out to 2.4 Å resolution. Data were corrected for absorption, LP factor and decay. Scaling each of the two native data sets to the derivative yielded R_F = 8.8% and 8.9% respectively. Scaling the two native data sets yielded R_F = 4.9%.

A difference Patterson map based on the averaged native and derivative data using all reflections with $F > 3\sigma$, (about two thirds of the total number of reflections) shows a single prominent heavy-atom site. A least-squares refinement of this site is in progress. Following this we plan to calculate an SIR map.

02.1-07 THE STRUCTURE OF THE RUBREDOXIN FROM DESULFOVIBRIO GIGAS. By M. FREY, G. PEPE and L.C. SIEKER, M. BRUSCHI, J. LE GALL, CRMC2, Campus de Luminy, case 913, 13288 Marseille cedex 9, France – Laboratoire de Chimie Bactérienne, 13274 Marseille cedex 9, France.

Rubredoxins are small proteins (M.W. 6000 DLTS.) which work in electron transfer systems of micro-organisms such as sulfate reducing bacteria. The active center is a single iron atom bonded tetrahedrally to a "cluster" of four cysteine residues.

A 2 Å resolution E.D. map of the rubredoxin from Desulfovibrio Gigas (RBDG), has been derived from the amplitudes of RBDG and phases of the rubredoxin from Desulfovibrio Vulgaris (RBDV) (Adman et al., J. Mol. Biol. (1977) 112, 113). The atomic model has been easily constructed thanks to the interactive graphics program *Bilder* (R. Diamond).

The three rubredoxins RBDG, RBDV and from Clostridium Pastorianum (RBCP) (Watenpaugh et al., J. Mol. Biol. (1979) 131, 509) do show substantial variations in their chemical sequences while their 3-D models resemble each other ; the structural differences concern the nature and the distribution over the surface of most of the charged residues.
The results of the first stages of the refinement and structural comparisons will be presented.

02.1-08 AN INTERIM REPORT ON THE THREE-DIMENSIONAL STRUCTURE ANALYSIS OF RABBIT PLASMA TRANSFERRIN. BY B. Gorinsky, P. F. Lindley, A. Mydin, D. Moss and J. Watson, Department of Crystallography, Birkbeck College, Malet Street, London, WC1E 7HX, UK.

Plasma transferrin is the key protein in the iron metabolism of vertebrates. The physiological significance of this glycoprotein lies in its central role in the cyclic process whereby iron derived from the catabolism of haemoglobin is conserved by its almost quantitative return to haemopoietic tissue. Transferrin also participates in the regulation of iron absorption and protects against iron toxicity.

Transferrin is a single-chain protein of molecular weight ca. 80,000, with two specific iron (III) binding sites. The metal protein complex is stabilised by the concomitant binding of one (bi)carbonate anion per iron atom. At physiological pH and oxygen tension the effective affinity constants of the metal sites are $\sim 10^{22}$ M^{-1}, precluding spontaneous dissociation of iron. Rapid iron transfer to cells is affected by reversible binding of the protein to specific membrane receptors.

Rabbit plasma transferrin crystallises in space group $P4_12_12$ (or enantiomorph) with $a = b = 127.4(3)$ and $c = 145.4(3)$ Å, and one molecule per asymmetric unit. The native crystals are grown within the temperature range 4-8 °C since at higher temperatures they are unstable. Approximately 70% of the crystal volume is occupied by solvent. Heavy-atom derivatives (mercuric-chloride, potassium chloroplatinate and uranyl acetate) have been prepared by soaking the native crystals in solutions of heavy-atom reagents in the mother liquor. X-ray diffraction intensity data for the native crystals and these three derivatives have been collected on a four-circle diffractometer. The method of isomorphous replacement